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## Hydrogen-Antihydrogen Interactions\*

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The interaction potential between hydrogen and antihydrogen is obtained by a variational calculation. A potential maximum is found, but its peak is below the dissociation limit. A classical calculation shows that the cross section for total annihilation decreases monotonically from  $31a_0^2$  at 0.01 eV to  $4a_0^2$  at 20 eV.

Interest in the atomic interactions involving antimatter has been aroused by the analysis of bubble-chamber reactions and by recent cosmological speculation concerning the possible presence of equal amounts of koinomatter and antimatter in the universe. Various authors<sup>1-4</sup> have pointed out that the rate of proton-antiproton annihilation in a system containing atoms or antiatoms may be considerably larger than in a system with just baryons and leptons. We will show that the study of the interactions between atoms and antiatoms presents some exacting and fascinating problems for the quantum chemist.

Consider a collision between neutral hydrogen and antihydrogen atoms. As the distance  $R$  between the proton and antiproton is reduced from "infinity," the binding energy of the electron and positron is reduced. As  $R \rightarrow 0$ , the interaction of each lepton with the two baryons is that of a dipole with decreasing moment. Since a dipole of arbitrarily small moment cannot bind an electron or positron, the system is unstable at small separations and both leptons will be emitted. There are critical separations  $R_{P_1}$  and  $R_F$  below which it is energetically more favorable for the leptons to leave the baryons, either as positronium ( $R < R_{P_1}$ ) or as a free pair ( $R < R_F$ ). Because of the binding energy of positronium,  $R_{P_1}$  is greater than  $R_F$ .

For slow collisions a simple adiabatic model

can be constructed. If, during the collision, the baryon separation becomes less than  $R_{P_1}$ , the leptons will be emitted as positronium. Since the binding energy of the lepton pair is now 6.8 eV, in the contrast to the 27.2 eV initially, the nuclear kinetic energy must be reduced by at least 20.4 eV. Hence if the initial kinetic energy is less than 20.4 eV, a bound state of protium will be formed. If the leptons escape while  $R$  is close to  $R_{P_1}$ , they will leave with little kinetic energy and the protium will be formed in one of the highest states consistent with energy conservation. This means a principal quantum number of 24 or 23. The levels of different  $l$  and  $m$  will be populated with roughly equal probability. After formation, the protium will lose energy by radiation or further collisions until annihilation occurs from a level with small  $n$  and  $l$  values. In this model  $R_F$  plays no role since by the time the nuclear separation reaches  $R_F$ , both leptons will have left. In the absence of further collisions the positronium will also suffer annihilation shortly after its formation.

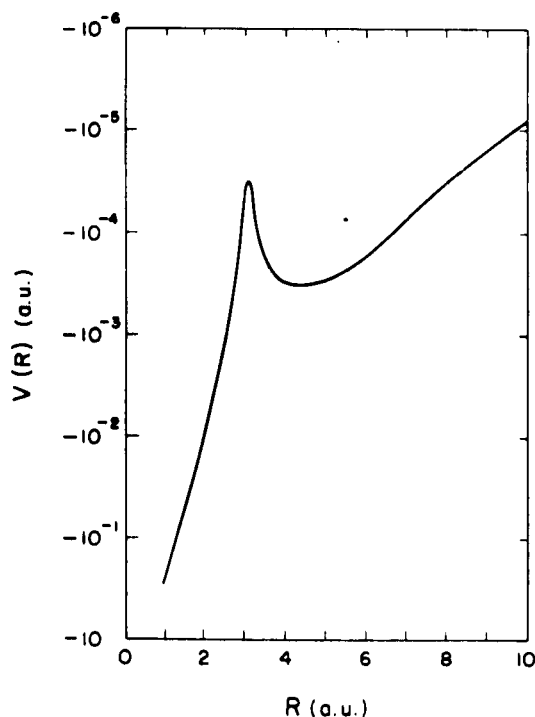
The annihilation cross section then depends only on the probability that  $R$  will become smaller than  $R_{P_1}$  at some time during the collision. Morgan and Hughes<sup>1</sup> estimated this probability with the assumption that the  $H-\bar{H}$  interaction is completely attractive. However, Puget<sup>2</sup> has shown that there may be a potential barrier since the

TABLE I. Energy of the H- $\bar{H}$  system with the nuclei at a fixed separation  $R$ .

$R$ (a.u.)	H- $\bar{H}$ interaction energy (a.u.)	$e^- - e^+$ binding energy (a.u.)
0.975	-0.277 201	0.001 560
1.0	-0.257 076	0.007 076
1.5	-0.055 216	0.138 549
2.0	-0.010 219	0.260 219
2.5	-0.001 244	0.351 244
3.0	-0.000 040	0.416 707
3.05	-0.000 033	0.422 165
3.10	-0.000 031	0.427 451
3.15	-0.000 039	0.432 579
3.5	-0.000 165	0.464 451
4.0	-0.000 301	0.500 301
5.0	-0.000 280	0.550 280
6.0	-0.000 154	0.583 487
10.0	-0.000 008	0.750 008

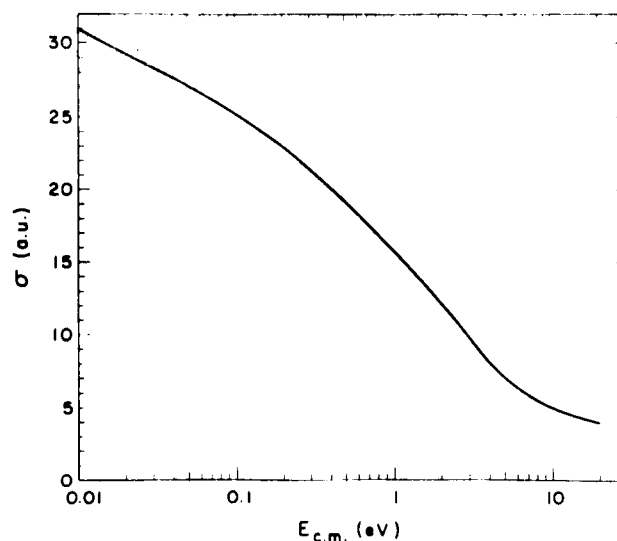
overlap of the lepton charge clouds leads to a repulsive interaction, in contrast to the attractive interaction produced for H-H. Using simple wave functions, Puget obtained a barrier of height 0.8 eV near  $1.8a_0$ . Such a barrier would clearly reduce the annihilation cross section significantly.

We have therefore calculated the H- $\bar{H}$  interaction by the variational method using a trial wave function with up to 75 configurations. Each configuration is made up from a product of orbitals,

FIG. 1. Interaction energy between H and  $\bar{H}$ .TABLE II. The H- $\bar{H}$  interaction energy at  $R=3.1$  a.u.

No. of terms in the wave function	Interaction energy (a.u.)
25	+0.000 700
47	+0.000 097
60	+0.000 034
75	-0.000 031

which are either Slater orbitals based on one of the nuclei or standard elliptical orbitals<sup>3</sup> based on both nuclei. The nonlinear orbital parameters, one for each Slater orbital and two for each elliptical orbital, were optimized to give the lowest energy with a wave function of 21 or 25 terms. The results of the 75-term calculation are shown in Table I and Fig. 1. At large  $R$  the potentials shows the attractive Van der Waals interaction, and at small  $R$  the  $p-\bar{p}$  Coulomb interaction produces a strong attraction. Between these regions there is a peak at 3.089 a.u., as determined by a cubic spline curve fitted through the points in Table I. The height of the peak is  $3.1 \times 10^{-5}$  a.u. (0.85 meV) below the dissociation limit. The binding energy of the lepton pair reduces to almost zero at 0.975 a.u., suggesting that  $R_{ps} \approx 0.96$  a.u. The rate of convergence of the calculation can be judged from Table II. It should be noted that in the 60-term calculation the energy at 3.1 a.u. was slightly higher than the dissociation limit. Thus, it was necessary to go to the 75-term function in order to demonstrate that the

FIG. 2. Cross section for the formation, with subsequent annihilation, of protium and positronium in H- $\bar{H}$  collisions.

potential maximum does not represent a barrier to zero-energy collisions with zero angular momentum.

The cross section for the formation of positronium and protium pairs, calculated using the adiabatic model together with classical trajectories, is shown in Fig. 2. The cross section decreases monotonically from  $31a_0^2$  at 0.01 eV to  $4a_0^2$  at 20 eV. These results should be accurate over the higher energies in this range, but quantum effects on the nuclear motion may influence the results at low energies.

The maximum in the  $H-\bar{H}$  potential is probably a feature common to all interaction potentials between neutral atoms and antiatoms. This suggests the possibility that for some pairs the potential at the maximum might be greater than the dissociation energy, thus providing a potential barrier which could keep matter and antimatter apart. This could perhaps give some support to the recent speculation<sup>6</sup> that ball lightning is caused by the congregation of large amounts of antimatter in the atmosphere. Preliminary studies on  $He-\bar{H}$ , with 7-term wave functions, reveal a small barrier which will probably disappear in

more accurate calculations. Our results for systems in which one or other atom is charged show no potential barriers.

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<sup>1</sup>D. L. Morgan and V. Hughes, *Phys. Rev. D* **2**, 1389 (1970).

<sup>2</sup>J. L. Puget, CERN Report No. TH1201, 1970 (unpublished), and *Nature (London)*, *Phys. Sci.* **230**, 173 (1971).

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<sup>4</sup>See also A. S. Wightman, *Phys. Rev.* **77**, 521 (1950).

<sup>5</sup>J. C. Browne and F. A. Matsen, *Phys. Rev.* **135**, A1227 (1964).

<sup>6</sup>D. E. T. F. Ashby and C. Whitehead, *Nature (London)*, *Phys. Sci.* **230**, 180 (1971).